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H_2 Generation in the Early Universe Governs the Formation of the First Stars

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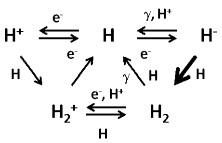
The chemistry of the early universe is seemingly simple since it involves only hydrogen and helium in various forms. The first stars formed out of this primordial gas after the "dark ages" several hundred million years after the Big Bang. How this happened in detail is one of the most exciting questions in astrophysics. It has long been realized that the formation of molecular hydrogen plays a key role in this scenario as it serves as an effective coolant at temperatures below 10^4 K. The most efficient mechanism for H_2 production under the conditions prevailing during this epoch is the associative detachment (AD) of hydrogen [Eq. (1)].

$$H^- + H \rightarrow H_2 + e^- \quad (1)$$

In a recent publication in the journal *Science* Kreckel et al. determined the rate coefficient for this key reaction as a function of the collision energy in a merged-beam apparatus.[1] The quality of the results makes is possible to accurately simulate the development of the primordial gas and to derive a much more precise picture of the formation of the first stars, in particular how much the gas must cool prior to star formation and how much gas is needed,[2] in other words, how heavy the new stars are.



Scheme 1. Network of chemical reactions producing H_2 in the early universe. The rate of formation by associative detachment (thick arrow) has been determined recently with high accuracy thus allowing for a more precise picture of the formation of the first stars.

The network of reactions involving hydrogen in the early universe is depicted in Scheme 1. Helium is in a neutral state and does not actively participate. The factor crucial for cooling the primordial gas, molecular hydrogen, is predominantly formed in a two-step process from atomic hydrogen by radiative association (RA) of an electron and by associative detachment (AD) [Eq. (1)]. Alternatively it can be formed by charge transfer in $H_2^+ + H$ collisions. However, this route is only significant at even earlier times when the cosmic microwave background temperature is higher and H^- is efficiently destroyed by photodetachment. Neglecting therefore this reaction, the net formation rate of H_2 in the epoch of early star formation is determined by the fractional ionization (i.e. the H^+/H ratio) of the gas, which controls the rate of the first reaction step (AD), the rate coefficient of which has now been determined by Kreckel et al.[1]

Experimental values for thermal AD rate coefficients $\alpha(T)$ of Equation (1) had been determined previously in flowing afterglow experiments over a rather limited temperature range (250–350 K),[3–5] not relevant for the simulation of the much hotter primordial gas. Calculations of the AD rate coefficient using scattering theory[6–9] along the attractive $X^2\Sigma_u^+$ potential arrive at largely differing values all diverging from the experimental values by a factor of 2–3 but with significant deviations among the theoretical values at elevated temperatures. The situation is now changed with the experimentally determined rate coefficients reported by Kreckel et al. In their experiment a beam of H^- was prepared and accelerated to roughly 10 keV. Photons from a high-power laser were used to detach the electron from a portion of the H^- to form the co-propagating H-atom beam. A slight acceleration of the ions by an additional field determines the collision energy for Equation (1). H_2 formed in the beam was monitored by electron stripping in high-energy collisions in a helium gas cell and subsequent detection of the H_2^+ product. Even though the determination of the energy-dependent rate coefficient $\alpha(E)$ from these measurements contains eight sources of error, the corresponding total error is limited to only 25%. Thermal rate coefficients $\alpha(T)$ were derived by thermal averaging of the measurements in the energy range $E/k = 0.1$–10^5 K.[1b]

On the basis of the much more accurate $\alpha(T)$ values cosmological simulations were carried out by Kreckel and coworkers to determine the evolution of the primordial gas. As can be seen from Scheme 1 the reactions of six species must be followed during the simulations, e^-, H^+, H, H^-, H_2^+, and H_2. Because of conservation of charge and number of hydrogen nuclei, the number of species in the simulation reduces to four. Since H^- and H_2^+ reach equilibrium very rapidly on the time scale of the simulations, their abundance was calculated under the assumption of instantaneous equilibrium. As a result, the evolution of only two species had to be treated explicitly. The simulations show that H_2 is formed efficiently by the AD reaction [Eq. (1)] owing to the high abundance of electrons. Its abundance reaches a constant value which depends critically on $\alpha(T)$ and the gas density. At a maximum H_2 abundance of 2.5 parts per thousand the cloud

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cools down to roughly 300 K. At these lower temperatures HD is a much better coolant than H_2 and must be considered even though the D/H ratio is only 2.6×10^{-5}. The HD abundance reaches a value of about 1 ppm by means of an efficient D–H exchange in $D^+ + H_2$ collisions. As a result, the cloud cools even further to a minimum temperature below 200 K. This is the environment in which the gas cloud collapses and the first stars form.

Owing to the much more accurate AD rate coefficient $\alpha(T)$, the uncertainty in the minimum cloud temperature is now substantially reduced. Therefore, the uncertainty of the corresponding characteristic mass of a first star is reduced by a factor of 10. These stars generate the first heavy elements out of their H/He gas. The development of this enrichment process depends on the mass of the first stars, and therefore a better understanding of star formation in the early universe is linked to the cosmological development leading to today's universe. It is discussed by Volker Bromm[10] that even the formation of the first galaxies might be affected by the AD rate coefficient. According to the current standard model of cosmological structure formation, the first stars emerge in small dark-matter halos, and one way to form galaxies is the composition of a large system of these stars. As a consequence, also the first galaxies might have been cooled down to lower temperatures and thus the masses of these stars could be smaller. These predictions can be tested by the James Webb Space Telescope (JWST) which will be launched in 2014. While this instrument will not be able to detect individual primordial stars, it might detect the color of clusters of these stars which also depends on the mass of the individual stars and the associated cooling process that led to their formation.

As it turns out, the cosmological development of our universe is governed by a simple network of reactions involving hydrogen. In particular the H_2 formation rate steers the development of the first stars and potentially the first galaxies. It is intriguing how a single microphysical process can have such far-reaching and large-scale cosmological implications. The current work by Kreckel et al. demonstrates how today's high-power computer simulations can be used for astrophysical predictions. Aided by a sensitivity analysis, the dominant processes can be identified for which precise experiments can be carried out. The theoretical predictions can be tested through observations and the astrophysical picture comes into sharper focus. It is this interplay between laboratory work, theory, and observations which helps us to uncover the secrets of our universe.

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